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Bill Calhoon " Application of Turbulence Models in Reacting Flows" **(Statement A)**

APPLICATION OF TURBULENCE MODELS IN REACTING FLOW

W. H. CALHOON, JR.
SPARTA, INC.
AIR FORCE RESEARCH LAB
EDWARDS AFB, CA

ARL MSRC PET SHORT COURSE ON
TREATMENT OF TURBULENCE MODELS IN
COMPLEX HIGH PERFORMANCE CFD APPLICATIONS,
16 - 17 MAR. 1998

OUTLINE

1. INTRODUCTION
2. OBJECTIVES
3. WHAT IS A "COMPLEX" REACTING FLOW?
4. FLOW MODELING : STEADY VS. UNSTEADY
5. REACTING FLOW EQUATIONS
6. TURBULENCE-CHEMISTRY INTERACTION MODELING
7. SAMPLE PROBLEM

1. INTRODUCTION: APPLICATION OF CFD TO REACTING FLOW

- **REQUIRES CHARACTERIZATION OF THE INTERACTION OF TURBULENCE AND CHEMISTRY**

- **TURBULENT COMBUSTION MODELING:**

  1) IS AN ENTIRE FIELD OF RESEARCH

  2) HAS BEEN THE SUBJECT OF INTENSE RESEARCH FOR ~ 25 YEARS

  3) MOST OF RESEARCH RESTRICTED TO:

     - LOW SPEED FLOWS
     - SMALL MEAN PRESSURE VARIATIONS
     - SIMPLE CONFIGURATIONS

KEY FEATURES OF TURBULENT REACTING FLOW

- **TURBULENT STIRRING:**
  - A PROCESS OF STRETCHING INTERMATERIAL AREA BETWEEN DIFFERENT FLUIDS (E.G., FUEL AND OXIDIZER)
  - CHARACTERIZED BY SCALAR LENGTH SCALE REDUCTION
- **MOLECULAR MIXING:**
  - THE PROCESS OF DIFFUSION OF SUBSTANCES ACROSS INTERMATERIAL AREA (E.G., MOLECULAR DIFFUSION)
- **FLUIDS MAY BE WELL STIRRED BUT NOT MOLECULARLY MIXED:**
  - CRUDE EXAMPLE: MIXING OF OIL AND WATER
- **COMBUSTION ONLY OCCURS WHEN REACTANTS ARE MOLECULAR MIXED**

2. OBJECTIVES

1) PROVIDE A "TIP OF THE ICEBERG" INTRODUCTION TO THE FIELD OF TURBULENT COMBUSTION

2) BRIEFLY COVER TWO MODELS APPLICABLE TO "COMPLEX" FLOWS

3) PROVIDE REFERENCES FOR SELF STUDY

3. WHAT IS A "COMPLEX" TURBULENT REACTING FLOW?

- <u>CHARACTERISTICS OF A "COMPLEX" REACTING FLOW:</u>
  - MULTIPLE SOURCES OF REACTANTS AND FUEL STREAMS
  - NONUNIFORM COMPOSITIONS IN THE FUEL STREAMS
  - CHEMICAL NONEQUILIBRIUM
  - HIGH SPEED FLOWS
    1) COMPRESSIBILITY EFFECTS
    2) LARGE PRESSURE VARIATIONS
    3) SHOCK WAVE HEATING
    4) HEATING DUE TO VISCOUS ENERGY DISSIPATION
  - COMPLEX MIXING
    1) SHOCK-SHEAR LAYER INTERACTIONS
    2) SEPARATED/RECIRCULATING FLOWS

CHARACTERISTICS OF A "COMPLEX" REACTING FLOW, CONT'D

- **THESE COMPLEX CHARACTERISTICS ELIMINATE TURBULENT COMBUSTION MODELS BASED ON:**

  1) **MIXTURE FRACTION FORMULATIONS**
     - **E.G., TWO STREAM CONFIGURATIONS**

  2) **INFINITE/FAST CHEMISTRY ASSUMPTIONS**

  3) **TABULARIZED FORMULATIONS**
     - **E.G., LAMINAR FLAMELET MODEL**

  4) **REDUCED FORMS OF THE ENERGY EQUATIONS**
     - **E.G., LOW SPEED, ~ CONSTANT PRESSURE FLOWS**

EXAMPLE OF A "COMPLEX" REACTING FLOW: MISSILE EXHAUST PLUMES

- **SIGNATURES IMPORTANT TO MISSILE DEFENSE SYSTEMS:**

  - **TYPING, TRACKING AND INTERCEPTOR AIMPOINT SELECTION**

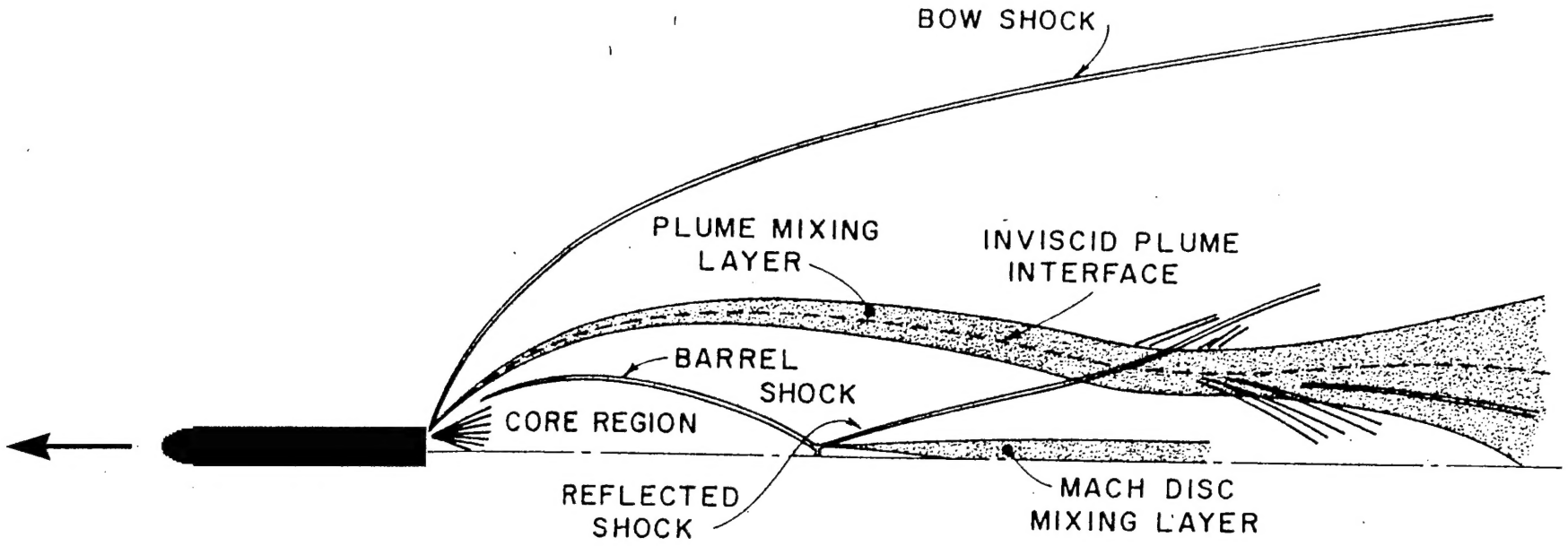
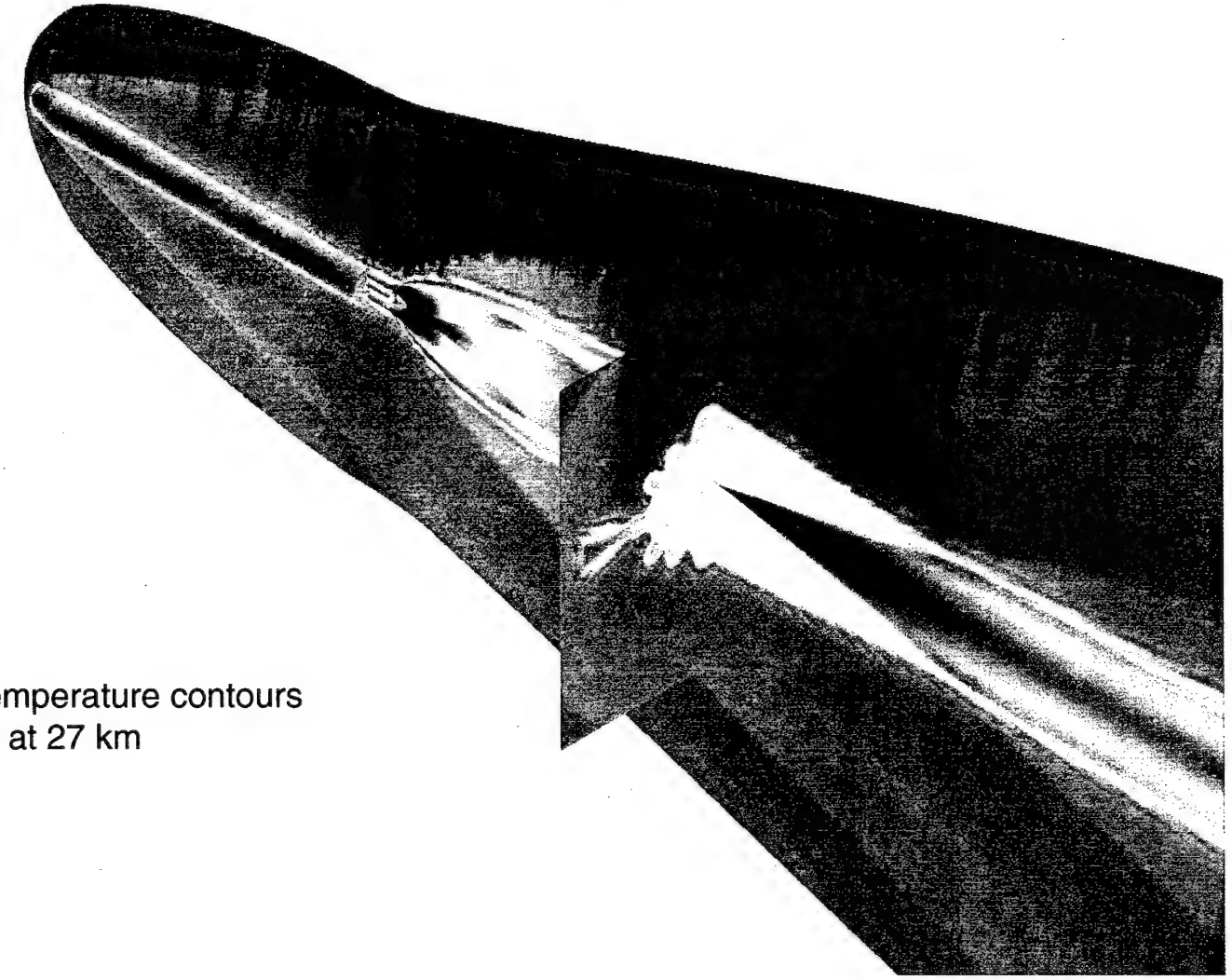


Fig. 1 Schematic of viscous/inviscid structure in plume nearfield.

EXAMPLE OF A "COMPLEX" REACTING FLOW: MISSILE EXHAUST PLUMES



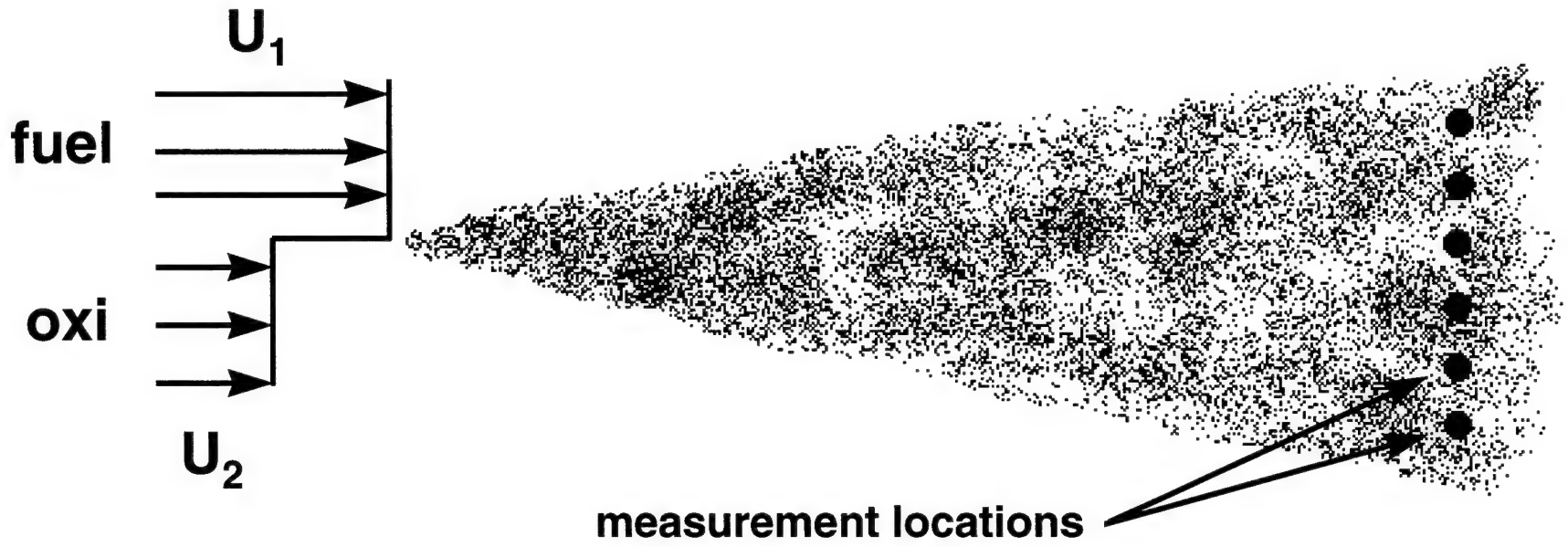
Titan II Temperature contours
at 27 km

4. FLOW MODELING : STEADY STATE VS. UNSTEADY STATE

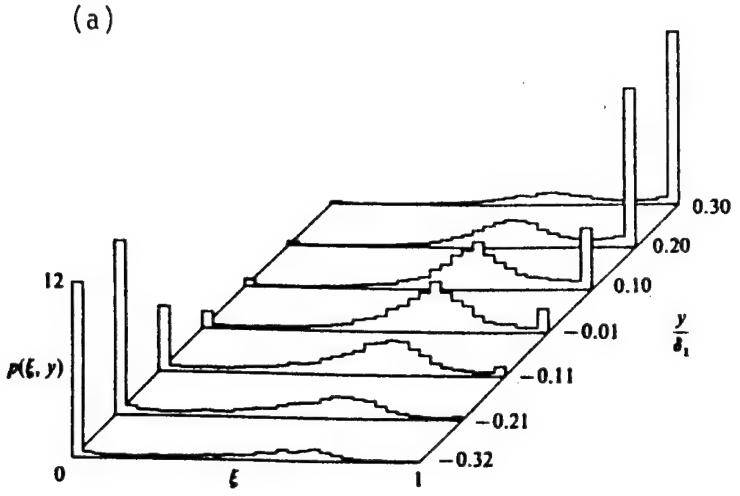
- **STEADY STATE VS. UNSTEADY**
  - TURBULENCE BY DEFINITION IS UNSTEADY
  - UNSTEADY SIMULATION METHODS PREFERABLE
- **STEADY STATE METHOD:**
  - REYNOLDS AVERAGED NAVIER-STOKES (RANS)
- **UNSTEADY METHODS:**
  - UNSTEADY RANS
  - LARGE-EDDY SIMULATION (LES)

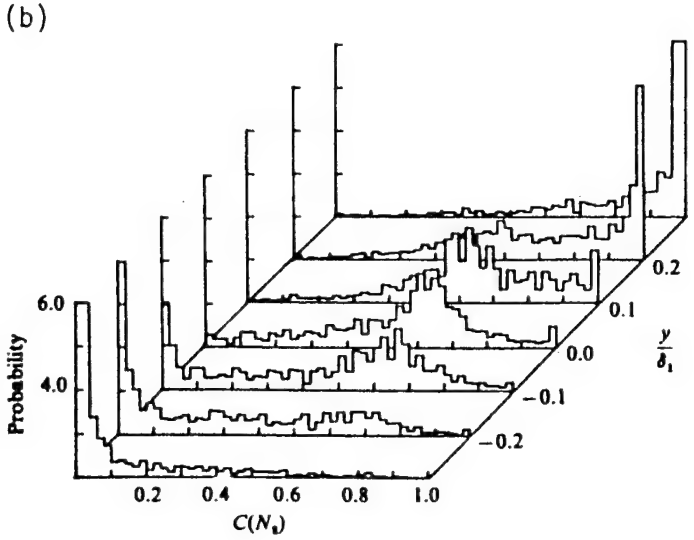
STEADY STATE VS. UNSTEADY

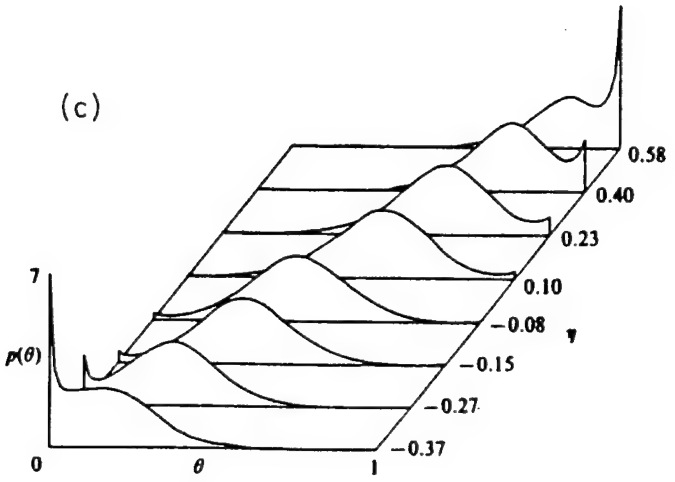
- **STEADY STATE METHODS LIMITED BY TURBULENT TRANSPORT MODELS FOR SCALARS**
  - **EXAMPLE : NONREACTING SHEAR LAYER MIXING**



SHEAR LAYER MIXING CHARACTERISTICS







Mixing layer normalized fuel probability density functions in the cross stream direction (a) liquid, Re = 23,000, (b) gas, Re = 25,000, (c) steady state calculation (Broadwell, J.E. and Mungal, M.G., 1991)

STEADY STATE VS. UNSTEADY

- **UNSTEADY METHODS:**
  - GOOD REPRESENTATION OF SCALAR TURBULENT TRANSPORT
  - HIGH RESOLUTION REQUIRED
  - COSTLY TIME ACCURATE SIMULATION REQUIRED
  - LES MODELS FOR COMPLEX FLOWS IMMATURE
- **STEADY STATE METHODS:**
  - LOWER RESOLUTION REQUIREMENTS
  - CONVERGENCE ACCELERATION TECHNIQUES APPLICABLE
  - THE ONLY ALTERNATIVE FOR MANY COMPLEX FLOWS
  - POOR REPRESENTATION OF TURBULENT TRANSPORT PRODUCED BY CURRENT MODELS

5. REACTING FLOW EQUATIONS

- **EQUATION SET (GAS PHASE):**
  - MASS, MOMENTUM, ENERGY AND SPECIES CONSERVATION
  - SUPPLEMENTED WITH STATE EQUATIONS

- **MASS, MOMENTUM AND ENERGY EQUATIONS THE SAME AS FOR NONREACTING EXCEPT:**
  - ADDITION HEAT FLUX TERM IN ENERGY EQUATIONS:

$$q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{k=1}^{K} Y_k h_k V_{k,j} + q_j^R$$

  - MOLECULAR PROPERTIES (VISCOSITY, THERMAL CONDUCTIVITY) ARE A FUNCTION OF THE LOCAL MIXTURE

SPECIES CONSERVATION AND STATE EQUATIONS

- **SPECIES CONSERVATION:**
  - $$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_j Y_k}{\partial x_j} = -\frac{\partial \rho V_{k,j} Y_k}{\partial x_j} + \dot{w}_k$$
  - $$Y_k = \rho_k / \rho \quad , \quad \sum_{k=1}^{k} \rho_k = \rho \quad , \quad \dot{w}_k = f(\rho, Y_k, T)$$
- **STATE EQUATIONS:**
  - $$p = \rho R^o T \sum_{k=1}^{K} \frac{Y_k}{W_k}$$
  - $$h = e + \frac{p}{\rho} = e + R^o T \sum_{k=1}^{K} \frac{Y_k}{W_k} = \sum_{k=1}^{K} Y_k \left[\Delta h_k^o + \int_{T^o}^{T} c_{p,k}(T') dT' \right]$$
  - $$c_{p,k}(T) = \sum_{n=0}^{N} a_{n,k} T^N$$

RANS SPECIES AND STATE EQUATIONS

- **VARIABLE DECOMPOSITION:** $\phi = \overline{\phi} + \phi' = \tilde{\phi} + \phi''$

- **SPECIES CONSERVATION:**

  - $$\frac{\partial \overline{\rho}\tilde{Y}_k}{\partial t} + \frac{\partial \overline{\rho}\tilde{u}_j\tilde{Y}_k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\overline{\rho} D_K \frac{\partial \tilde{Y}_k}{\partial x_j}\right] - \frac{\partial}{\partial x_j}\left[\overline{\rho u_j'' Y_k''}\right] + \overline{\dot{w}}_k$$

- **STATE EQUATIONS:**

  - $$\overline{p} = \overline{\rho} R^o \sum_{k=1}^{K} \frac{\tilde{T}\tilde{Y}_k}{W_k} + R^o \sum_{k=1}^{K} \frac{\overline{\rho T'' Y_k''}}{W_k}$$

  - $$\tilde{e} + R^o \sum_{k=1}^{K} \frac{\tilde{T}\tilde{Y}_k}{W_k} + \frac{1}{\overline{\rho}} R^o \sum_{k=1}^{K} \frac{\overline{\rho T'' Y_k''}}{W_k} = \sum_{k=1}^{K} \tilde{Y}_k \Delta h_k^o + \tilde{h}^s$$

  - $$\tilde{h}^s = \frac{1}{\overline{\rho}} \sum_{k=1}^{K} \overline{\rho Y_k \int_{T^o}^{T} c_{p,k}(T')dT'} = f\left(\overline{\rho T'' Y_k''}, \overline{\rho T''^{n+1} Y_k''}\right)$$

RANS UNCLOSED TERMS

- **TURBULENT TRANSPORT:** $\overline{\rho u_j'' Y_k''}$
  - **MODELED BY:**
    1) **GRADIENT DIFFUSION :**

$$\overline{\rho u_j'' Y_k''} = -\frac{\overline{\rho}\, \nu_T}{Sc_T} \frac{\partial \tilde{Y}_k}{\partial x_j}$$

    2) **SECOND ORDER CLOSURE**

- **SCALAR MOMENTS:**
  - **MEAN REACTION RATE:** $\overline{\dot{w}_k}$
  - **TEMPERATURE-SPECIES CORRELATIONS:** $\overline{\rho T'' Y_k''}$, ..., ...
  - **MODEL THE SINGLE POINT JOINT PDF OF** ρ **,** T **AND** Y_k **:** $P(\rho, T, Y_k)$
  - $$\overline{\dot{w}_k} = \int_0^\infty \int_0^\infty \int_0^1 \ldots \int_0^1 \dot{w}_k P(\rho', T', Y_k') dY_1' \ldots dY_k' d\rho' dT'$$

6. TURBULENCE-CHEMISTRY INTERACTION MODELING

- **INTERACTION OF TURBULENCE AND CHEMISTY CONTAINED IN THE SINGLE POINT PDF** $P(\rho, T, Y_k)$
- $P(\rho, T, Y_k)$ **REPRESENTS THE COMBINED EFFECTS OF:**
  - **TURBULENT TRANSPORT (LARGE AND SMALL SCALE)**
  - **MOLECULAR DIFFUSION**
- **ESTABLISHED MODELS FOR** $P(\rho, T, Y_k)$**:**
  - **LAMINAR MODEL**
  - **EDDY DISSIPATION CONCEPT**

LAMINAR MODEL FOR THE PDF

- **LAMINAR MODEL FOR** $P(\rho,T,Y_k)$**:**
  - $P(\rho,T,Y_k) = \delta(\rho-\overline{\rho})\delta(T-\tilde{T})\sum_{k=1}^{K}\delta(Y_k-\tilde{Y}_k)$
  - $\overline{\dot{w}_k} = \overline{\dot{w}_k}(\overline{\rho},\tilde{T},\tilde{Y}_k)$
  - $\overline{\rho T'' Y_k''} = 0$

- **COMMENTS:**
  - **CAN BE IN ERROR BY AN ORDER OF MAGNITUDE**
  - **WIDELY USED AS A FIRST APPROXIMATION**
  - **CAN GIVE GOOD RESULTS WHEN FLUCTUATIONS ARE UNIMPORTANT**
  - **NO GENERAL CRITERIA OF THE APPLICABILITY RANGE OF THE MODEL**

EDDY DISSIPATION CONCEPT (EDC)

- **OBSERVATIONS:**
  - REACTIONS ONLY OCCUR WHEN SPECIES MOLECULARLY MIXED
  - MICROSCALE STRUCTURES, WHERE MOLECULAR EFFECTS ARE IMPORTANT, ONLY OCCUPY A SMALL FRACTION OF THE TOTAL FLUID VOLUME
- **EDC MODEL:**
  - FLUID CONSISTS OF FINE SCALE STRUCTURES AND SURROUNDING FLUID
  - CHEMICAL REACTIONS ONLY OCCUR IN THE FINE SCALES
  - FINE SCALES ASSUMED HOMOGENEOUSLY MIXED
  - FINE SCALES REPRESENT BY A "PERFECTLY STIRRED REACTOR" (PSR)
  - $$P(\rho,T,Y_k) = \delta(\rho-\hat{\rho})\delta(T-\hat{T})\sum_{k=1}^{K}\delta(Y_k-\hat{Y}_k) + \delta(\rho-\rho^*)\delta(T-T^*)\sum_{k=1}^{K}\delta(Y_k-Y_k^*)$$

EDDY DISSIPATION CONCEPT (EDC)

- **MEAN REACTION RATE:**
  - $\overline{\dot{w}}_k = A_{EDC}\,\dot{f}\,\Delta m_k$
  - $\dot{f}$ - **FLOW RATE TO FINE SCALES PER UNIT MASS**
  - Δm_k - **MASS PER UNIT VOLUME CHANGE IN FINE SCALE SPECIES**
  - A_{EDC} - **MODEL PARAMETER**

- **MOST ELEMENTARY FORM FOR FAST CHEMISTRY:**
  - $F + rO \rightarrow P$
  - $\varphi_p = W_F / rW_O$
  - $\varphi_{st} = (W_F + rW_O) / W_F$
  - A_{EDC} **= CONSTANT**

$$\overline{\dot{w}}_F = -A_{EDC}\overline{\rho}(\tilde{\varepsilon} / \tilde{k}) \min\left[\tilde{Y}_F, \tilde{Y}_O \varphi_{st}\right]$$

$$\overline{\dot{w}}_O = -A_{EDC}\overline{\rho}(\tilde{\varepsilon} / \tilde{k}) \min\left[\tilde{Y}_F / \varphi_{st}, \tilde{Y}_O\right]$$

$$\overline{\dot{w}}_P = -\overline{\dot{w}}_F \varphi_p$$

EDDY DISSIPATION CONCEPT (EDC)

- **MORE GENERAL FORMS OF EDC MODEL:**
  - A_{EDC}, $\dot{f}$ - ESTIMATED FROM ENERGY CASCADE THEORY
  - CAN INCLUDE REVERSIBLE REACTIONS
  - Δm_k FROM PSR CALCULATION FOR FINITE RATE CHEMISTRY
  - CAN FORMULATE AN EXTINCTION MODEL

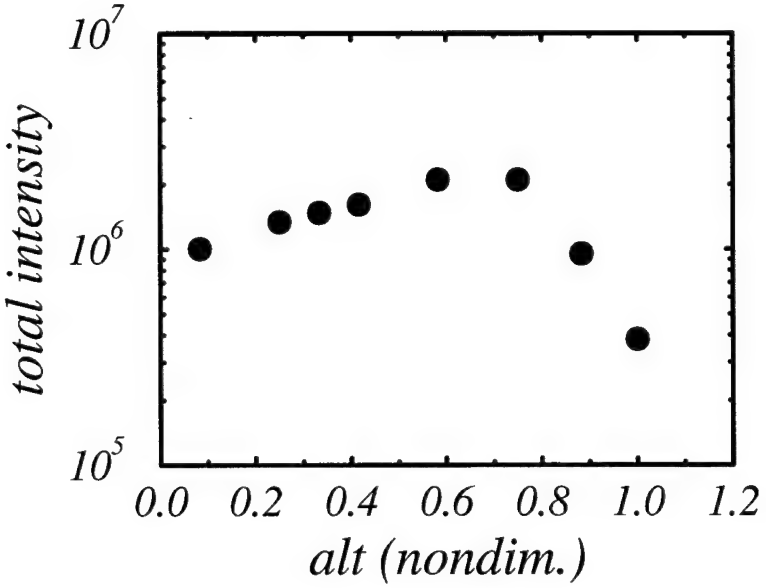
- **COMMENTS:**
  - VERY INEXPENSIVE FOR FAST CHEMISTRY
  - HIGH SENSITIVITY TO MODEL PARAMETER, A_{EDC}, AND INFLOW TURBULENCE
  - GOOD FOR RUNNING PERMUTATIONS AROUND A KNOWN CALIBRATION POINT

EXAMPLE OF THE IMPORTANCE OF TURBULENCE CHEMISTRY INTERACTIONS: MISSILE PLUME AFTERBURNING CESSATION

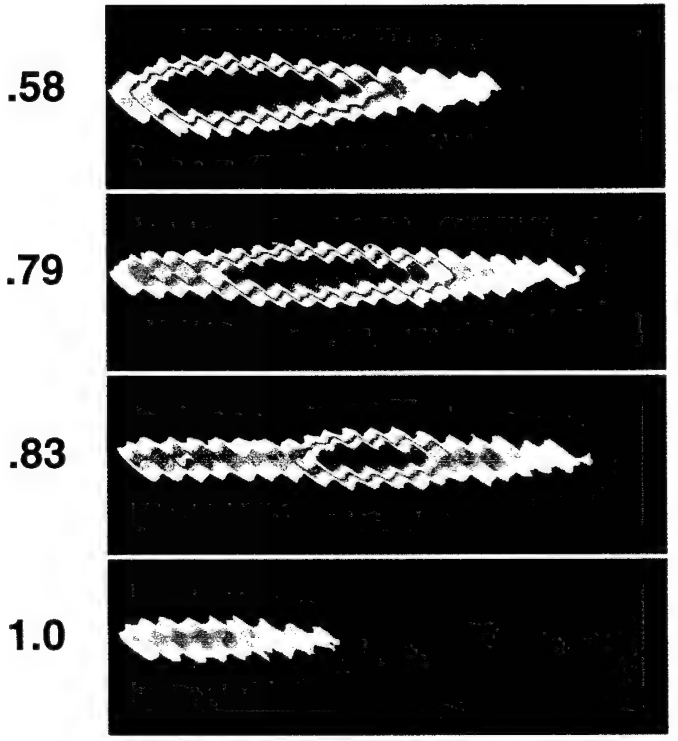
AFTERBURNING CESSATION IMPORTANT TO:

- SURVEILLANCE SENSOR DEVELOPMENT
  - DETERMINATION OF NOISE EQUIVALENT TARGET THRESHOLD
  - SENSOR DYNAMIC RANGE
- MISSILE TYPING
- PLUME-TO-HARDBODY HANDOVER AND AIMPOINT SELECTION ALGORITHMS

EXAMPLE OF RAPID CESSATION EVENT



TOTAL INTENSITY AS A FUNCTION OF ALTITUDE



SPATIAL RADIANT INTENSITY

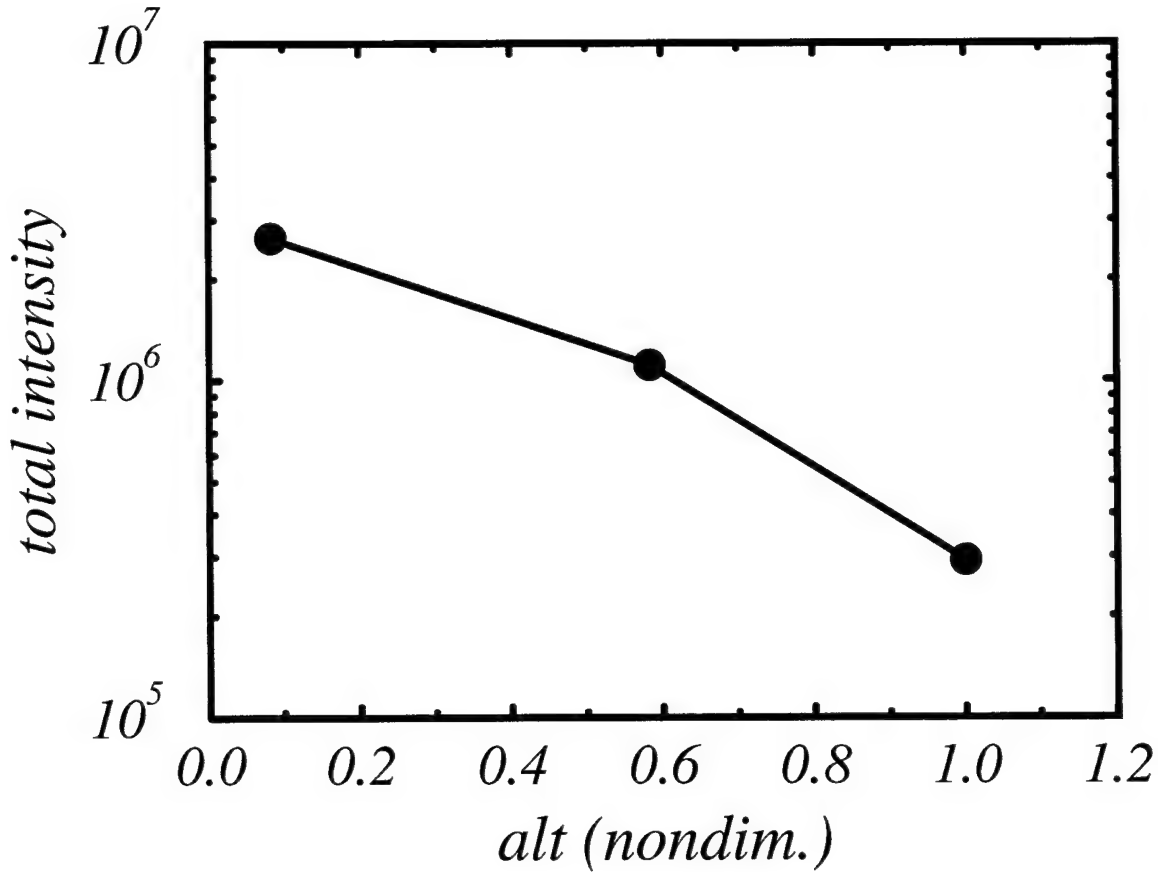
POSSIBLE MECHANISMS FOR RAPID AFTERBURNING CESSATION

- **SHEAR LAYER RELAMINARIZATION (VELOCITY MATCHING):**
  - AFTERBURNING INHIBITED BY LACK OF TURBULENT MIXING
- **DAMKOHLER NUMBER EFFECT:**
  - DAMKOHLER NUMBER IS RATIO OF MIXING AND CHEMICAL TIME SCALES
  - LARGE SCALE TURBULENT MIXING COOLS PLUME FASTER THAN AFTERBURNING HEATS THE PLUME (LOW DAMKOHLER NUMBER)
- **CLASSICAL FLAME EXTINCTION MECHANISM:**
  - HIGH TURBULENT MIXING RATES AT THE SMALL SCALES CAUSES LOCAL FLAME EXTINCTION AND EVENTUAL AFTERBURNING CESSATION

COMPUTATIONAL METHODOLOGY

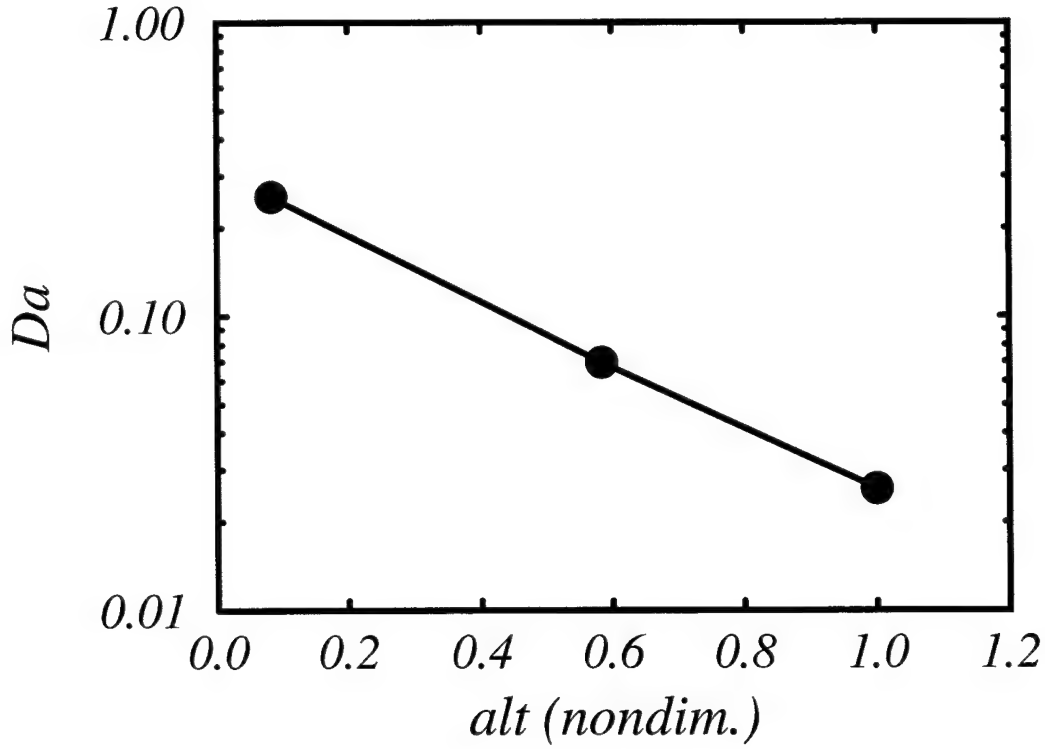
- **SIMULATIONS ACCOMPLISHED USING THE "GASP" CODE:**
  - GENERAL AERODYNAMIC SOLVER FOR COMPRESSIBLE REACTING FLOWS
  - INCLUDES MODERN, WIDELY ACCEPTED TURBULENCE MODELS
  - DRAWBACK: NEGLECTS THE EFFECT OF TURBULENCE-CHEMISTRY INTERACTIONS
  - FINITE RATE/EXTINCTION VERSION OF EDC MODEL IMPLEMENTED TO ACCOUNT FOR TURBULENCE-CHEMISTRY INTERACTIONS
- **MISSILE MODELING:**
  - SIMULATE THE ENTIRE MISSILE BODY, BASE AND PLUME
  - ASSUME ONLY AXISYMMETRIC BODY CONFIGURATION

PREDICTED TOTAL RADIANT INTENSITY

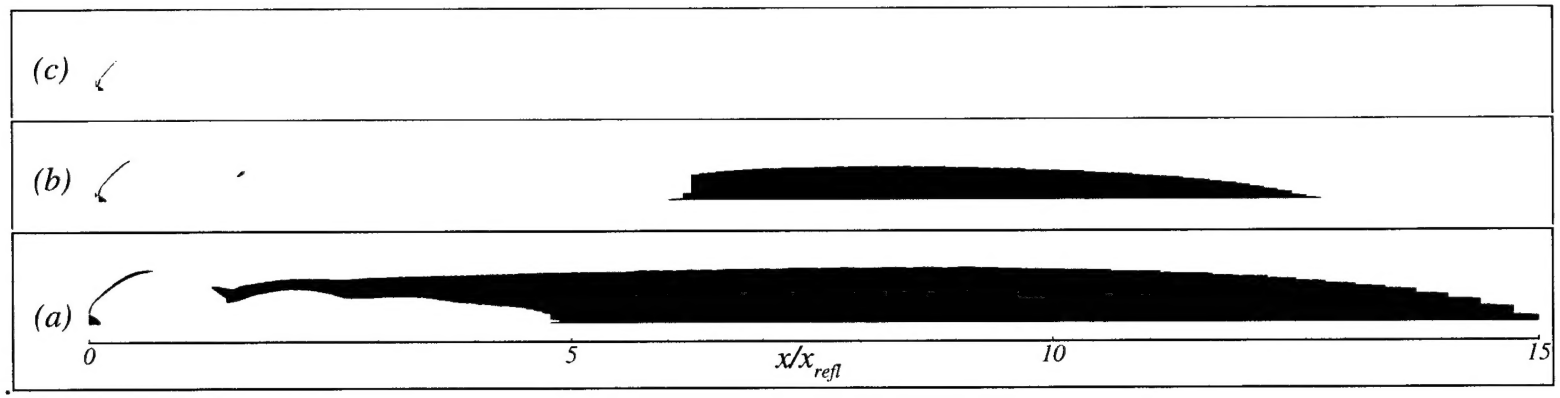


DAMKOHLER NUMBER VARIATION WITH ALTITUDE ENGINE MODELS

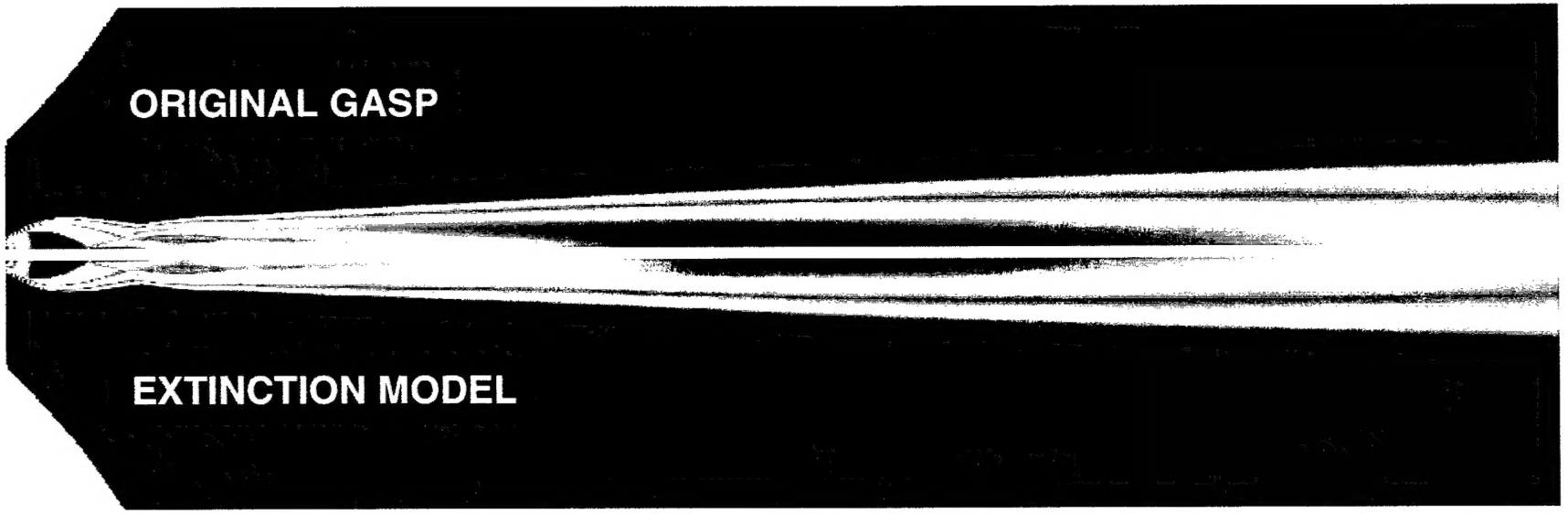
$$Da = \tau_{mix}/\tau_{chem}$$

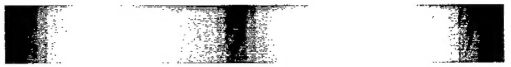


CONTOUR PLOT OF THE EXTINCTION MODEL BINARY SWITCH

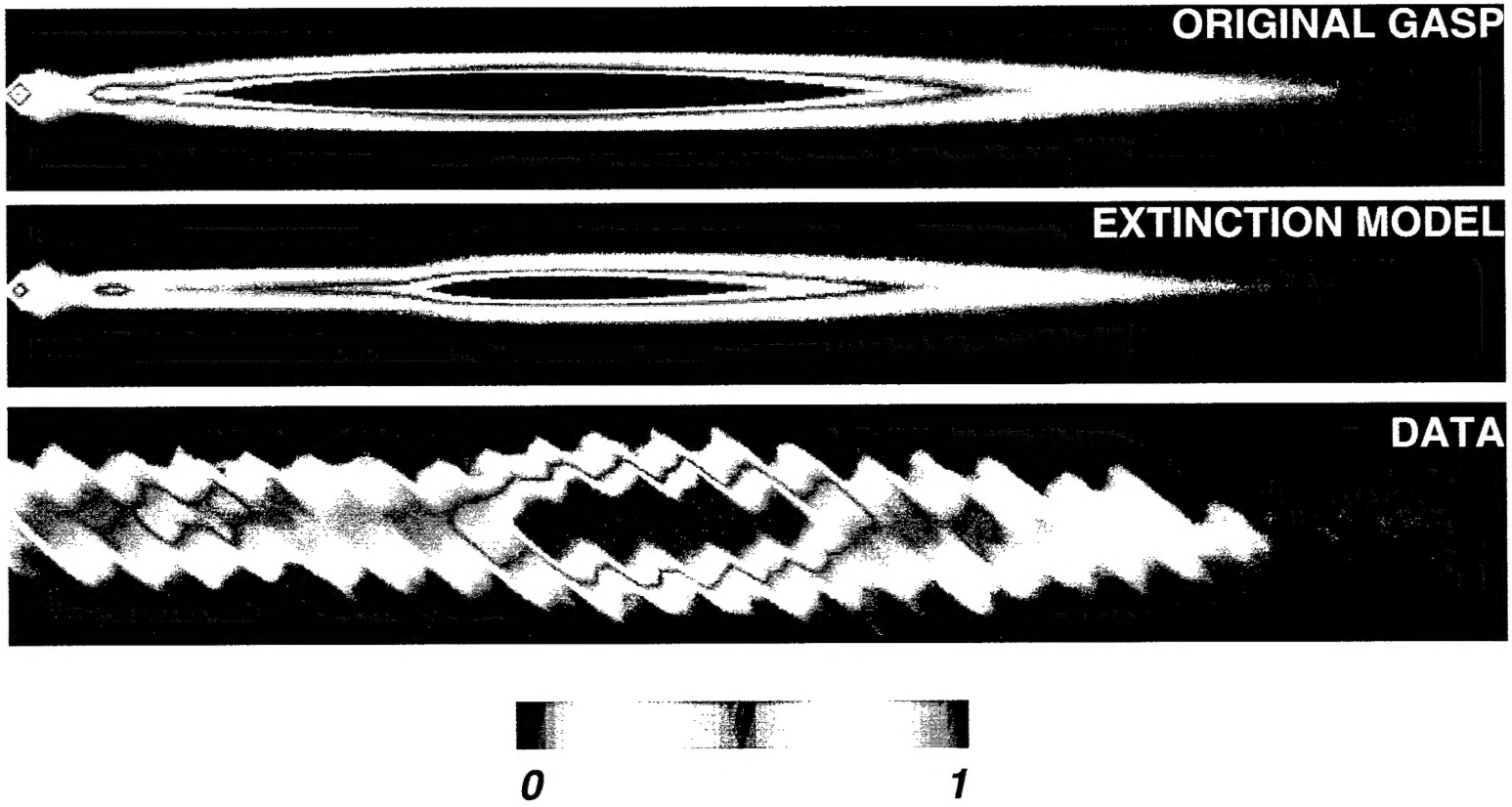


COMPARISON OF TEMPERATURE CONTOURS USING EXTINCTION MODEL





EFFECT OF EXTINCTION MODEL ON SPATIAL RADIANT INTENSITY PREDICTIONS DURING THE CESSATION EVENT



CONCLUSIONS

- PROPERLY ACCOUNTING FOR TURBULENCE-CHEMISTRY INTERACTIONS IN REACTING FLOW SIMULATIONS CAN BE CRITICAL

- TURBULENT COMBUSTION MODELS HAVE BEEN DEVELOPED FOR COMPLEX FLOWS

- TURBULENT COMBUSTION MODELS EFFICIENT ENOUGH FOR ROUTINE APPLICATION